Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.80e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.71e-01

Confidence level: 5.00e-01

Nearest Neighbors from the Training Set

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DKA 24
Measured: 9.13e-02
Predicted: 2.17e-02

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2-(Ethylamino)-2-oxoethyl benzoate
Measured: 5.79e-03
Predicted: 2.07e-02

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Glycine, N-benzoyl-, methyl ester
Measured: 8.80e-02
Predicted: 2.38e-02

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2-(Methylamino)-2-oxoethyl benzoate
Measured: 1.92e-02
Predicted: 2.35e-02